AR201-13311

Luella Hill
11/23/01 10:04 AM

To: NCIC HPV@EPA
cc:
cc:
Subject: HPV registration number

John Heinze <jheinze@johnadams.com> on 11/21/2001 10:39:36 AM

To: NCIC OPPT/DC/USEPA/US@EPA, Rtk Chem/DC/USEPA/US@EPA
cc:

Subject: HPV registration number

On June 8, 1999 the Council for LAB/LAS Environmental Research (CLER) filed a letter of commitment to sponsor six (6) chemicals in the HPV Challenge Program. On November 30, 1999 CLER added three (3) chemicals to that list, bringing the total to nine (9) chemicals being sponsored in the Program.

As the data was being accumulated on those nine (9) chemicals, it became clear that one of those chemicals, although made using technology similar to the other eight, is obtained at a different point in the process than the others. In addition, it is manufactured by only one company member of CLER. It was decided that the chemical should be sponsored by that company in a separate filing from the others.

This submission is for that chemical Benzene, C6 -12 alkyl derivatives, CAS # 68608-80-0. The sponsoring company is Huntsman Corporation. John Adams Associates managed the development of the robust summary and the assessment plan. The robust summary was prepared using the IUCLID Data Set software and is being submitted in PDF format. The assessment plan is also being submitted in PDF format.

The assessment plan is also being submitted to the industry electronic database at the US HPV Chemical Tracking System website.

I am the contact for this submission and for comments. If there are any questions, please do not hesitate to contact me.

--John E. Heinze, Ph.D.
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Final Final Robust Summary Doc Final Final Akylate Top Assesmen

AR201-13311A

Assessment Plan for Benzene, C6-12 Alkyl Derivatives in Accordance with the USEPA High Production Volume Challenge Program

Prepared for

Huntsman Corporation

November 8, 2001

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WASHINGTON, D.C.
NEW YORK
BRUSSELS
PARIS
SAN FRANCISCO

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I. INTRODUCTION

The High Production Volume (HPV) Challenge Program is a voluntary initiative of the US chemical industry to complete hazard data profiles for approximately 2800 HPV chemicals as identified on the US Environmental Protection Agency's (USEPA) 1990 Toxic Substances Control Act (TSCA) Inventory Update Rule (IUR). In the US, HPV chemicals are those that are manufactured or imported in quantities greater than 1 million pounds per year. The hazard data to be provided in the program are those that meet the requirements of the Screening Information Data Set (SIDS) Program. SIDS, which has been internationally agreed to by member countries of the Organization for Economic Cooperation and Development (OECD), provides the basic screening data needed for an initial assessment of the physical-chemical properties, environmental fate, and adverse human and environmental effects of chemicals. The information for completing the SIDS can come from existing data or may be generated as part of the HPV Challenge Program. Once the available studies are identified or conducted, "robust summaries" are prepared.

The USEPA, industry, and non-governmental organizations (NGOs) are unified in their commitment to minimize the numbers of animals tested in the HPV Challenge Program whenever it is scientifically justifiable. One approach toward this consideration is to evaluate closely related chemicals as a group, or category, rather than solely as individual chemicals. This approach takes advantage of structure activity relationships (SARs), which is based on the understanding that chemicals with similar structures often have similar and/or predictable characteristics and behavior in the environment and in mammalian systems. The use of categories and SARs is encouraged by USEPA in the HPV Challenge Program. Appropriate use of SARs can allow for a more efficient evaluation of the available data and significantly reduce the number of animals required for testing.

Huntsman Corporation (Huntsman) has agreed to assemble and review available public and private toxicological data, develop and provide an assessment plan for the sponsored material and conduct additional research, including testing when necessary, for one alkylated benzene mixture (hereafter referred to as an "Alkylate Top"). While Huntsman is not proposing this material as part of a category approach *per se*, as a mixture it is appropriate to review the pertinent data of the principal constituents using SAR as a means to help characterize the Alkylate Top's properties and characteristics.

This assessment plan is the result of Huntsman's efforts and provides a summary and analysis of the available data, and identifies any data gaps in the SIDS data profile. Section II of this assessment plan provides a characterization of the sponsored Alkylate Top production process and use patterns. Section III reviews the methods used in the collection of published and unpublished data. Section IV reviews the evaluation of data quality. Section V is an in-depth evaluation of the available data, first for the Alkylate Top itself, then for its principal constituents and for Linear Alkylbenzene (LAB). Section VI is a summary of the Alkylate Top and constituents properties. Section VII presents the conclusions regarding data availability and identifies data gaps in the SIDS profile.

II. IDENTIFICATION OF THE SPONSORED MIXTURE

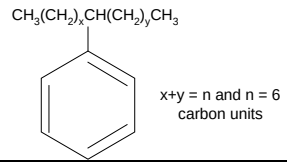
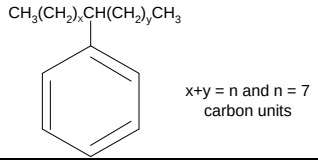
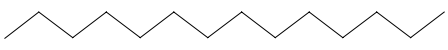
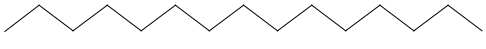
A. Production Process

Huntsman is sponsoring Benzene, C6-12 alkyl derivatives (CAS #68608-80-0) in the USEPA HPV Challenge Program. This "Alkylate Top" is a mixture of aromatic and aliphatic hydrocarbons derived as a low boiling point co-product from the LAB manufacturing process. This LAB production process entails the partial conversion of *n*-paraffins to internal *n*-olefins by catalytic dehydrogenation. The resulting mixture of *n*-paraffins and *n*-olefins is selectively hydrogenated to reduce diolefins and fed into an alkylation reactor together with benzene (in excess) and hydrofluoric acid as a catalyst in the Friedel-Crafts reaction. The Alkylate Top results from an intermediate distillation cut prior to the isolation of the final LAB product and serves to remove impurities with a lower boiling point than LAB. Following the removal of the Alkylate Top, a final distillation removes commercial detergent grade LAB as the distillate.

This production process results in an alkylated benzene mixture, the Alkylate Top, which is comprised primarily of C9 and C10 alkylbenzenes and C14 and C15 *n*-paraffins (alkanes). Within each group, the C9-LAB predominates the alkylbenzenes and the C14 predominates the paraffins. Table 1 shows representative structures of the constituents that make up the Alkylate Top mixture. The alkylbenzene constituents are secondary alkyl chain materials (e.g., C9-LAB and C10-LAB) than can be attached to the benzene ring at the 2, 3, 4, or 5 positions. However, the primary alkylbenzenes (e.g., nonyl- and decylbenzene) are chemical isomers and would be expected to have properties essentially similar to the secondary alkylbenzenes. Therefore, data for the primary alkylbenzenes are utilized where appropriate.

TABLE 1

Representative Structures of the Constituent Compounds of the Alkylate Top

COMPOUND	(Relative %)	CAS NUMBER	REPRESENTATIVE STRUCTURE
C9-LAB	45	--	
C10-LAB	10	--	
n-Tetradecane	35	629-59-4	
n-Pentadecane	3	629-62-9	

B. Use Patterns and Exposure potential

Currently, 100% of the sponsored Alkylate Top is sold into the marine diesel fuel market as a blend stock for viscosity control. This is the only active use of the material. During production, it is sufficient for workers to employ standard personal protective equipment to minimize exposure. During use, very limited human and environmental exposure to marine diesel fuel is expected, given its destruction during the combustion process. Environmental exposure may occur if the diesel fuel is spilled in transit and thus presents the same limited exposure potential as other types of fuel spills. Because the Alkylate Top is only a component of the fuel, the potential for significant exposure would be even further reduced.

III. COLLECTION OF PUBLISHED AND UNPUBLISHED DATA

Huntsman Corporation contributed in-house data on physical-chemical properties, environmental fate and transport, ecotoxicity, and mammalian toxicity for the sponsored Alkylate Top mixture. To supplement these data, literature searches were conducted of on-line databases (e.g., Hazardous Substances Databank [HSDB], Registry of Toxic Effects of Chemical Substances [RTECS], and Aquatic Toxicity Information Retrieval [AQUIRE]), standard scientific data compendia (e.g., *CRC Handbook of Chemistry and Physics* and *The Merck Index*), and other published sources (e.g., International Uniform Chemical Information Database [IUCLID]). The literature search encompassed the Alkylate top itself, as well as its principal constituents and the structural similar primary alkylbenzenes. The sum total of the in-house studies, reference books, and literature searches of on-line databases was the identification of available data for key properties of the sponsored Alkylate Top and related materials.

IV. EVALUATION OF DATA FOR QUALITY AND ACCEPTABILITY

The collected data were reviewed for quality and acceptability following the general USEPA and OECD SIDS guidance and the systematic approach described by Klimisch et al. These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. The Klimisch approach specifies four categories of reliability for describing data adequacy. These are:

1 **Reliable without Restriction:** Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.

2 **Reliable with Restrictions:** Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.

3 **Not Reliable:** Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.

4 **Not Assignable:** Includes studies or data in which insufficient detail is reported to assign a rating, e.g., listed in abstracts or secondary literature.

Only those studies which are deemed reliable for current HPV Challenge Program purposes are included in the data set for this assessment plan. Reliable studies include both categories rated 1 (Reliable without restriction) and 2 (Reliable with restrictions). Studies rated 3 (Not reliable) were not used. Studies rated 4 (Not assignable) were used when professional judgment deemed it appropriate as part of a weight-of-evidence approach. Finally, some older studies were not included if they had been superceded by more recent studies rated 1.

Some of the available data were from study reports conducted by either outside contract laboratories or in-house industry laboratories. These study reports followed standard procedures for testing of physical-chemical properties, environmental fate and transport, aquatic toxicity, and mammalian toxicity. The most recent studies were conducted under GLP provisions. Additional data were obtained from the published, peer-reviewed, scientific literature. Reliable data from all of these sources were incorporated into the data set as appropriate.

V. EVALUATION OF THE AVAILABLE DATA

All of the available data were compiled and robust summaries were prepared according to the format recommended by the USEPA and OECD. These summaries were then entered into the standard International Uniform Chemical Information Database (IUCLID) software and present the salient information from each of the reliable studies. All of the summaries are collected into a dossier that includes the sponsored Alkylate Top mixture as well as its principal constituents and structurally related materials. In addition, because the Alkylate Top is formed during the production process for LAB and its constituents include structural similarities, data for LAB are included. The dossier containing the robust summaries for the Alkylate top and related chemicals should be used in conjunction with this assessment plan.

Table A-1 in the Appendix to this assessment plan is a matrix of SIDS/HPV endpoints and the available data for the sponsored Alkylate Top and related materials. The table includes data for LAB as a benchmark for comparison. The materials are organized left to right in the table beginning with LAB, followed by the sponsored Alkylate Top, the principal constituents of the Alkylate Top mixture (pentadecane, tetradecane, and C10-LAB), and then the structurally similar primary C9 and C10 alkylbenzenes. Data drawn from the robust summaries are shown in the table for each endpoint when available. Endpoints for which specific data are not available are identified by "--" in the table. The data presented for LAB were obtained from a completed European dossier and risk assessment report (Revision June 1997). The extent to which each of the endpoints is adequately characterized by the available data is evaluated.

A. *Evaluation of the Available Data on the Alkylate Top*

Adequate data for key physical-chemical, environmental fate, acute ecotoxicity, and acute mammalian toxicity properties of the Alkylate Top are available. These data are summarized below.

Physical-Chemical Properties

Boiling point and water solubility information for the Alkylate Top material is available from Huntsman Material Safety Data Sheets. While the quality of these data could not be adequately assessed, the boiling point values are consistent with the expected values compared to LAB.

Environmental Fate

The ultimate biodegradability (i.e., mineralization) of the Alkylate Top and other alkylated materials was evaluated in 1980 by Monsanto using a shake flask CO_2 evolution test similar to the standard ASTM practice. Periodic removal and titration of a barium hydroxide solution was used to determine the CO_2 evolved. Results show a mean of 46% degradation (range 43-51%) after 35 days. This represents a moderate biodegradation rate, primarily due to the degradation of the paraffin and alkylbenzene components. It should be noted that the composition of the tested material was 29% paraffin, 44% alkylbenzene and 24% indanes. Due to improvements in the manufacturing process, modern Alkylate Top consists of approximately 40% paraffin and 60% alkylbenzene and virtually no indanes. Since the high percentage of the less degradable indanes would depress the overall biodegradation rate of the mixture, it is likely that this study actually represents an under-prediction of the degradation of the modern Alkylate Top. Therefore, the available data indicate that modern Alkylate Top will biodegrade in the environment.

Aquatic Toxicity

The aquatic toxicity of the Alkylate Top was determined by ABC Laboratories in 1981 using a standard fish toxicity test under GLP conditions. Fathead minnows were exposed to five nominal concentrations ranging from 100 to 1000 mg/L for 96 hours. Acetone was used as a solvent to assist in dissolving the test material to levels significantly over its water solubility limit (as evidenced by an oily film on the surface of all test solutions). No mortality or sublethal effects were observed and the 96-hour LC_{50} value was determined to be greater than 1000 mg/L.

Mammalian Toxicity

The acute toxicity of the Alkylate Top mixture has been evaluated in a series of studies conducted in the early and late 1970s by Younger Laboratories. Oral toxicity studies in rats were conducted in 1973 at a limit dose of 15,800 mg/kg, and were repeated in 1978 at a limit dose of 10,000 mg/kg. In both sets of studies, rats were given a single undiluted dose of L210L or L210H[*] (both CAS#68608-80-0) by gavage and observed for 14 days. No mortality was

[*] L210L and L210H are essentially the same material and no longer segregated.

observed in any of the studies at these doses, resulting in oral LD_{50} values greater than 15,800 mg/kg and 10,000 mg/kg.

Acute dermal studies were conducted at the same time as the oral studies. Undiluted L210L or L210H was applied to the intact skin of New Zealand albino rabbits for 24 hours and the rabbits were observed for 14 days. Results indicate acute LD_{50} values of greater than 5,010 mg/kg in both the earlier tests and greater than 2,000 mg/kg and 1,260 mg/kg for the L210L and L210H, respectively, in the later tests. Rabbits treated with higher doses (e.g., 7,940 mg/kg in the earlier tests, 5,010 mg/kg in the later tests) experienced mortality and gross visceral alterations during the studies.

Acute inhalation studies were also conducted by Younger Laboratories. For these tests, Sprague-Dawley albino male rats were exposed to vapor concentrations of L210L or L210H ranging up to 0.9 mg/L. Rats were held in 35 L exposure chambers with the test materials for 6 hours at 27 ºC, then removed and observed for 14 days. No mortality or other toxic signs were observed in any of the tests conducted.

In summary, adequate data are available for the sponsored Alkylate Top to characterize its acute mammalian toxicity. Results show that the Alkylate Top mixture is not acutely toxic at environmentally relevant levels. Single dose oral and inhalation studies result in no observable acute toxicity, and the dermal exposures result in acute toxicity only at extremely high levels. Therefore, it can be concluded that the Alkylate Top does not present an unreasonable acute risk to mammals.

Summary of the Available Data on the Alkylate Top

Adequate data exist to characterize the biodegradation, acute toxicity to fish, and acute toxicity to mammals of the sponsored Alkylate Top. These data demonstrate that the Alkylate Top will undergo substantial degradation in the environment and does not present an acute toxicity concern for fish or mammals.

Specific data are not available to characterize the Alkylate Top mixture's toxicity to aquatic invertebrates or to characterize the potential effects of long-term mammalian exposure. Therefore, the available environmental fate and toxicity data for the principal constituents of the mixture have been reviewed and evaluated in order to assist in the characterization of the Alkylate Top. Data for the structurally similar primary alkylbenzenes were also evaluated when data were available. Given the mixture's production in the LAB production process, comparison to the properties of LAB is also appropriate. This evaluation is summarized below.

B. *Evaluation of the Available Data on LAB and the Constituent Compounds*

As discussed above, the principal constituents of the Alkylate Top mixture are secondary alkylbenzenes (specifically, C9-LAB and C10-LAB) and paraffins (specifically, tetradecane and pentadecane).

Physical-Chemical Properties

As can be seen in Table A-1, the principal constituents and structurally related materials all have very similar and predictable physical-chemical properties. All have boiling points less than LAB, as is necessitated by the distillation process by which the Alkylate Top mixture and its constituents are produced. All of the constituents are of low to moderate volatility and very low water solubility. The reported log octanol/water partition coefficients are all very high and fall within a narrow range of 7.11 to 7.72. These data indicate similarity with the existing data for the Alkylate Top and LAB. While data on the physical-chemical properties of the Alkylate Top itself are limited, the data for the principal constituents show a consistency that allows for the estimation of properties for the sponsored mixture. Based on the sum of the information one can predict that the Alkylate Top will have a low to moderate volatility, low water solubility and high octanol/water partitioning.

Environmental Fate

Studies conducted on the Alkylate Top indicate that it biodegrades under environmental conditions. Available data for its constituents also indicate substantial biodegradation. As discussed above, the Alkylate Top used in the biodegradation study had a significant percentage of indanes (24%). Given that the data show substantial biodegradation for the paraffin and alkylbenzene components, and the lack of significant indane composition in the modern Alkylate Top, one would expect even greater biodegradation than the Alkylate Top study suggests.

Aquatic Toxicity

A study conducted on the Alkylate Top demonstrates that the mixture is not acutely toxic to fish even at concentrations enhanced via solvents to levels much greater than its solubility in water. Studies conducted on decylbenzene confirm that the material is not acutely toxic to fish or *Daphnia* at the water solubility limit. Furthermore, data for LAB also demonstrate no acute toxicity to fish, *Daphnia*, or algae at saturation. Exposure to enhanced concentrations using solvents also do not result in toxicity to algae and the EC50 for *Daphnia* is 1.1 mg/L – far above the solubility limit of LAB. Given the structural similarities between the Alkylate Top, LAB, and the constituent materials, one would expect that toxicity to fish, *Daphnia* and algae would be similar. Thus, no acute toxicity at the water solubility limit would be expected. Chronic aquatic toxicity data are not available, but environmental exposure is limited to spill situations and therefore chronic exposures are very unlikely.

Mammalian Toxicity

The acute toxicity of the Alkylate Top to mammals is adequately characterized. Data for all of the other endpoints are available for LAB, and the Alkylate Top is expected to show similar behavior. Acute toxicity data for pentadecane and a reported repeated dose value for tetradecane support the apparent lack of toxicity.

VI. SUMMARY OF THE AVAILABLE DATA

The sponsored Alkylate Top is a mixture of aromatic and aliphatic hydrocarbons derived as a low boiling point co-product from the LAB manufacturing process. Available data indicate that the Alkylate Top will biodegrade in the environment, will not be acutely toxic to aquatic organisms at its water solubility limit, and is not acutely toxic to mammals by the oral or inhalation routes of exposure. No acute effects were observed at relatively high doses following dermal exposures, although some effects were noted at extremely high dermal contact with the material. However, the use of Alkylate Top almost exclusively in auxiliary fuel significantly limits environmental and consumer exposure. The Alkylate Top manufacturing process is closed and workers can use personal protective equipment to effectively minimize risk. Data for LAB, the principal constituents of the mixture, and structurally related alkylbenzenes help to fill in any gaps in the characterization of the Alkylate Top.

VII. CONCLUSIONS

Given the availability of data for the key endpoints, the biodegradation potential, the lack of significant toxicity concerns, and the limited exposure potential, no further testing is deemed necessary to characterize the Alkylate Top mixture.

Table A-1
Summary of Data Available for the LAB Alkylate Top

Section	Description	Benzene C10-13 alkyl derivs. (LAB)	Benzene, C6-12 alkyl derivatives "Alkylate Top"	Pentadecane (C15 normal paraffin)	Tetradecane (C14 normal paraffin)	C10-LAB	Decylbenzene	Nonylbenzene
	CAS Number	**67774-74-7**	**68608-80-0**	**629-62-9**	**629-59-4**		**104-72-3**	**1081-77-2**
	Physical-Chemical Data							
2.1	Melting Point	< -70°C	--	10 C	6 C	--	-14 C	-24 C
2.2	Boiling Point	278-314°C	240-250 C	271 C	253 C	276-286 C 262-286 C **	300 C	282 C
2.4	Vapour Pressure	0.017 hPa *	--	0.0046 hPa	0.0155 hPa	--	0.0017 hPa	0.0076 hPa *
2.5	Octanol/Water Partition Coefficient (log)	7.5-9.12 *	--	7.72	7.2	7.5	7.35	7.11 *
2.6.1	Water Solubility	0.041 mg/L at 27°C 0.037 mg/L	< 1,000 mg/L	0.00008 mg/L	0.0022 mg/L	0.040 mg/L	0.0024 mg/L	0.035 mg/L *
	Environmental Fate and Pathways							
3.1.1	Photodegradation	< 1% after 14 days	--	$t_{1/2}$ = 7.1 hrs *	$t_{1/2}$ = 7.7 hrs *		$t_{1/2}$ = 7.5 hrs *	$t_{1/2}$ = 8.1 hrs *
3.1.2	Stability in Water	--	stable	--	--	--	--	--
3.5	Biodegradation	56-61% biodeg after 35 days 64-67% biodeg after 28 days	46% after 35 days	100% in seawater in 8 weeks; 75% degradation by sediment microbes in 8 days	100% in seawater in 8 weeks; Biodegrades easily	--	--	65% after 10 days; 72% degradation by sediment microbes in 8 days
	Ecotoxicity							
4.1	Acute/Prolonged Toxicity to Fish	No effects up to soluble limits LC_{50} > 1,000 mg/L with a solvent	LC_{50} >1,000 mg/L with a solvent	NOEC > 1240 ppm	NOEC > 2110 ppm	LC_{50} > Water Solubility (0.079 mg/L)	--	--
4.2	Acute Toxicity to Daphnia	No effects at saturated concentration (up to 0.041 mg/L); EC_{50} = 1.1 mg/L with a solvent	--	--	--	EC_{50} > 0.10 mg/L	--	--
4.3	Toxicity to Aquatic Plants (e.g., algae)	No effects up to soluble limits EC_{50} > 1,000 mg/L with a solvent	--	--	--	EC50 > 0.10 mg/L	--	--
	Toxicity							
5.1.1	Acute Oral Toxicity	LD_{50}(rat) > 5,000 mg/kg	LD_{50}(rat) >10,000; >15,800 mg/kg	--	--	--	--	--
5.1.2	Acute Inhalation Toxicity	LC_{50} > 1.82 mg/L LC_{50} = 71 mg/L	No toxic effects after 6 hours at concentrations of up to 0.9 mg/L	--	--	--	--	--
5.1.3	Acute Dermal Toxicity	LD_{50} > 2,000 mg/kg	LD_{50}(rabbit) >2000; >1,260; >5,010 mg/kg	--	--	--	--	--
5.1.4	Acute Toxicity by Other Routes	--	--	LD_{50}(i.v., mouse) = 3493 mg/kg	--	--	--	--
5.4	Repeated Dose Toxicity	NOEL = 102 mg/m^3 (inhalation) LOEL = 125 mg/kg (oral)	--	--	TD_{LO}(mice) = 9600 mg/kg for 20 weeks		--	--
5.5	Genetic Toxicity in-vitro (Bacterial test)	Negative	--	--	--	--	--	--
5.5	Genetic Toxicity in-vitro (Non-bacterial test)	Negative	--	--	--	--	--	--
5.6	Genetic Toxicity in-vivo	Negative	--	--	--	--	--	--
5.8	Toxicity to Reproduction	NOAEL (maternal) = 50 mg/kg NOAEL (fetal) = 50 mg/kg	--	--	--	--	--	--
5.9	Developmental Toxicity/Teratogenicity	NOAEL (maternal) = 125 mg/kg Not teratogenic	--	--	--	--	--	--

* Estimated Values
** Estimated data for C9-LAB based on regression analysis

AR201-13311B

IUCLID

DATA SET

Existing Chemical	**Benzene, C6-12 Alkyl Derivatives (CAS# 68608-80-0)**
Producer	
Company:	**Huntsman Corporation**
Creation date:	**May 2, 2001**
Prepared by	
Company:	**THE WEINBERG GROUP INC.**
Printing date:	**November 8, 2001**
Revision date:	
Date of last update:	**November 8, 2001**
Number of pages:	**44**

I U C L I D

D a t a S e t

Existing Chemical Substance ID: Atops

Producer Related Part
Company: The Weinberg Group Inc.
Creation date: 02–MAY–2001

Substance Related Part
Company: The Weinberg Group Inc.
Creation date: 02–MAY–2001

Printing date: 08–NOV–2001
Revision date:
Date of last Update: **08–NOV–2001**

Number of Pages: **44**

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA–Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC

1.0.1 OECD and Company Information

Name: Huntsman Corporation

03–OCT–2001

1.0.2 Location of Production Site

Remark: The production site is located in North America.
03–OCT–2001

1.0.3 Identity of Recipients

Remark: Not applicable
03–OCT–2001

1.1 General Substance Information

Substance type: organic
Physical status: liquid
Remark: Alkylate benzene mixture derived as a lower boiling point co–product from the LAB manufacturing process. Benzene, C6–12 alkyl derivs. (68608–80–0)
05–NOV–2001

1.1.1 Spectra

Remark: Not applicable
03–OCT–2001

1.2 Synonyms

Remark: Alkylate Top
22–OCT–2001

1.3 Impurities

CAS–No:
EINECS–No:
EINECS–Name:
Remark: Not specified
03–OCT–2001

1.4 Additives

CAS–No:
EINECS–No:
EINECS–Name:
Remark: Not specified
03–OCT–2001

1.5 Quantity

Quantity 1 000 – 5 000 tonnes
08–NOV–2001

1.6.1 Labelling

Labelling:
Remark: There are no specific labeling requirements for the alkylate top.
03–OCT–2001

1.6.2 Classification

Classification:
Class of danger:
R–Phrases:
Remark: There are no specific classification requirements for the alkylate top.
03–OCT–2001

1.7 Use Pattern

Type:
Category:
Remark: Greater than 95% of the alkylate top is used as auxiliary fuel.
03–OCT–2001

1.7.1 Technology Production/Use

Remark: Not applicable
03–OCT–2001

1.8 Occupational Exposure Limit Values

Type of limit:
Limit value:
Remark: No TLV’s have been established.
03–OCT–2001

1.9 Source of Exposure

Memo: Very limited potential for human or environmental exposure.
03–OCT–2001

1.10.1 Recommendations/Precautionary Measures

Remark: Use of appropriate personel protective equipment.
03–OCT–2001

1.10.2 Emergency Measures

Remark: Flush with water. Ventilate area. Wipe up or absorb on suitable material and shovel into appropriate container.
03–OCT–2001

1.11 Packaging

Memo: Product is available in tank cars and tank trucks.

03–OCT–2001

1.12 Possib. of Rendering Subst. Harmless

Type of destruction:

Remark: Flush with water
03–OCT–2001

1.13 Statements Concerning Waste

Memo: Dispose of waste in accordance with appropriate RCRA and local requirements.

03–OCT–2001

1.14.1 Water Pollution

Classified by:
Labelled by:
Class of danger:
Remark: Not required
03–OCT–2001

1.14.2 Major Accident Hazards

Legislation:
Substance listed:
Remark: As with all chemicals, avoid contact with skin, eyes or clothing.
03–OCT–2001

1.14.3 Air Pollution

Classified by:
Labelled by:
Number:
Class of danger:
Remark: Not required
03–OCT–2001

1.15 Additional Remarks

Memo: None
03–OCT–2001

1.16 Last Literature Search

Date of Search: 15–AUG–2001

03–OCT–2001

1.17 Reviews

Memo: None
03–OCT–2001

1.18 Listings e.g. Chemical Inventories

Additional Info: Listed on TSCA Inventory, Canadian DSL, and EINECS or ELINCS

03–OCT–2001

2.1 Melting Point

Value: < –70 degree C
Decomposition: no
Sublimation: no
Method: other: DIN 51 583
GLP: no data
Remark: No data specifying done as GLP, but presumed GLP based on reported use of DIN protocol.
Source: Wibarco 1993.
Test substance: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Reliability: (2) valid with restrictions
Reported in LAB Risk Assessment document citing a DIN protocol.
25–JUL–2001 (7)

Value: = 10 degree C
Method: other: no data
GLP: no data
Test substance: Pentadecane (C15 normal paraffin) (629–62–9)
Reliability: (2) valid with restrictions
Standard reference text.
22–OCT–2001

Value: = 6 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Tetradecane (C14 normal paraffin) (629–59–4)
Reliability: (2) valid with restrictions
Standard reference text.
02–NOV–2001 (11)

Value: = –14 degree C
GLP: no data
Source: Jeng 1992.
Test substance: Decylbenzene (104–72–3)
Reliability: (1) valid without restriction
25–JUL–2001 (26)

Value: = –24 degree C
GLP: no data
Source: Jeng 1992.
Test substance: Nonylbenzene (1081–77–2)
Reliability: (1) valid without restriction
25–JUL–2001 (26)

2.2 Boiling Point

Value: = 278 – 314 degree C at 1013 hPa
Decomposition: yes
Method: other: ASTM D 86
Year: 1989
GLP: no
Source: EniChem Augusta Industriale 1993.
Test substance: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Reliability: (2) valid with restrictions
Reported in LAB Risk Assessment document.
25–JUL–2001 (13)

Value: = 240 – 250 degree C
GLP: no data
Source: Huntsman MSDS 2000.
Test substance: Alkylate L–210 (Benzene, C6–12 alkyl derivatives; 68608–80–0)
Reliability: (4) not assignable
Data from MSDS but original study report not available for review.
25–JUL–2001 (22)

Value: = 271 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Pentadecane (C15 normal paraffin) (629–62–9)
Reliability: (2) valid with restrictions
Standard reference text.
01–NOV–2001 (11)

Value: = 253 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Tetradecane (C14 normal paraffin) (629–59–4)
Reliability: (2) valid with restrictions
Standard reference text.
01–NOV–2001 (11)

Value: = 276 – 286 degree C
Method: other: Internal laboratory analysis
GLP: no data
Remark: Normal boiling points at 1 atm for 2, 3, 4, and 5–phenyldodecanes.
Source: Huntsman 2001.
Test substance: C10–LAB
Reliability: (2) valid with restrictions
05–NOV–2001 (23)

Value: = 262 – 286 degree C
GLP: no
Method: Estimation of C9–LAB 2, 3, 4, and 5 phenyl isomers based on a regression analysis of the C10–C14 LAB positional isomer data.
Source: Rapko 2001.
Test substance: C9–LAB
Reliability: (2) valid with restrictions
08–NOV–2001 (34)

Value: = 300 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Decylbenzene (104–72–3)
Reliability: (2) valid with restrictions
Standard reference text.
01–NOV–2001 (11)

Value: = 282 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Nonylbenzene (1081–77–2)
Reliability: (2) valid with restrictions
Standard reference text.
01–NOV–2001 (11)

2.3 Density

Type:
Value:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

2.3.1 Granulometry

Type of distribution:

Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

2.4 Vapour Pressure

Value: = .0017 hPa at 25 degree C
Method: other (calculated)
GLP: no
Source: EPIWIN V.3.10
Test substance: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Reliability: (2) valid with restrictions
Standard EPA peer–reviewed database and estimation software.
25–JUL–2001

Value: = .0046 hPa at 25 degree C
GLP: no data
Source: Daubert 1989.
Test substance: Pentadecane (C15 normal paraffin) (629–62–9)
Reliability: (2) valid with restrictions
Cited in HSDB but original report not available for review.
25–JUL–2001 (42)

Value: = .0155 hPa at 25 degree C
GLP: no data
Source: Daubert 1989.
Test substance: Tetradecane (C14 normal paraffin) (629–59–4)
Reliability: (2) valid with restrictions
Cited in HSDB but original report not available for review.
02–NOV–2001 (10)

Value: = .0017 hPa at 25 degree C
GLP: no data
Source: Daubert 1989.
Test substance: Decylbenzene (104–72–3)
Reliability: (2) valid with restrictions
Cited in HSDB but original report not available for review.
02–NOV–2001 (10)

Value: = .0076 hPa at 25 degree C
Method: other (calculated)
GLP: no data
Source: EPIWIN V.3.10
Test substance: Nonylbenzene (1081–77–2)
Reliability: (2) valid with restrictions
Standard EPA peer–reviewed database and estimation software.
02–NOV–2001 (46)

2.5 Partition Coefficient

log Pow: = 7.5 – 9.12 at 25 degree C
Method: other (calculated): Fragment constants by Hansch and Leo
Year: 1979
GLP: no
Remark: The individual calculated values using the fragment constant method are 7.5, 8.04, 8.58, and 9.12 for LABs of alkyl chain length C10, C11, C12, and C13, respectively.
Source: Sherblom et al 1988; Hansch and Leo.
Test substance: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Reliability: (2) valid with restrictions
25–JUL–2001 (17) (41)

log Pow: = 7.72
Method: other (calculated): Extrapolated from Hutchinson et al
Year:
GLP: no data
Source: Coates et al 1985; Hutchinson et al 1980.
Test substance: Pentadecane (C15 normal paraffin) (629–62–9)
Reliability: (2) valid with restrictions
25–JUL–2001 (8) (24)

log Pow: = 7.2
Method: other (measured): Head space chromatographic method
Year:
GLP: no data
Source: Sangster 1989; Coates et al 1985.
Test substance: Tetradecane (C14 normal paraffin) (629–59–4)
Reliability: (1) valid without restriction
25–JUL–2001 (8) (40)

log Pow: = 7.35
Method: other (measured): Shake flask
Year:
GLP: no data
Source: Sangster 1989; Bruggeman et al 1982.
Test substance: Decylbenzene (104–72–3)
Reliability: (1) valid without restriction
01–NOV–2001 (5) (40)

log Pow: = 7.11
Method: other (calculated): EPIWIN V.3.10
Year:
GLP: no data
Test substance: Nonylbenzene (1081–77–2)
Reliability: (2) valid with restrictions
Standard EPA peer–reviewed database and estimation software.
25–JUL–2001

2.6.1 Water Solubility

Value: = .041 mg/l at 27 degree C
Qualitative: of very low solubility
Method: other: Monsanto method
GLP: yes
Remark: Gas chromatographical determination: aqueous solubility was reported as the sum of linear C9–13 alkylbenzene GC peak areas.
Source: Gledhill et al 1991.
Test substance: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Reliability: (1) valid without restriction
25–JUL–2001 (16)

Value: = .037 mg/l
GLP: yes
Method: Six mL of LAB were deposited on the top of approximately 700 mL of ultra–pure water in a reaction vessel. The solution was stirred and maintained at 20–23 degrees Celcius. After 96 hours, 100 mL aliquots were sampled and the water accommodated fraction determined.
Remark: The WAF were determined to be 0.037, 0.040, and 0.049 mg/L for LAB, Phenyl C–10, and Phenyl C–12, respectively. The total solubility seems to be independent of the number of components in the mixture, and therefore for a single compound, the final water concentration in saturated solutions will depend on the total number of isomers/homologues present in the mixture. Further, the relative composition of the saturated solutions differs from that observed for the mixture, these differences

seem to be regulated by a more complex mechanism than liphophilicity.
Source: Alonso et al 1999.
Test substance: Phenyl-C10 (C10 LAB) and LAB (67774-74-7)
Reliability: (1) valid without restriction
03-OCT-2001 (2)

Value: < 1000 mg/l
GLP: no data
Remark: Data listed in MSDS as < 0.1%.
Source: Huntsman 2000.
Test substance: Alkylate L-210 (Benzene, C6-12 alkyl derivatives; 68608-80-0)
Reliability: (4) not assignable
Data from MSDS but original study report not available for review.
03-OCT-2001 (22)

Value: = .00008 mg/l
Method: other: Extrapolated from Hutchinson et al
GLP: no data
Source: Coates et al 1985; Hutchinson et al 1980.
Test substance: Pentadecane (C15 normal paraffin) (629-62-9)
Reliability: (2) valid with restrictions
25-JUL-2001 (8) (24)

Value: = .0022 mg/l at 25 degree C
Method: other: Shake flask
Remark: Methods meeting current standards were used. Flasks were shaken gently for 12-hours, then allowed to sit at 25 plus or minus 0.1 degrees Celcius for another 24 hours to allow dispersed droplets to rise to the surface. Aliquots of 100 mL were removed and filtered through a 0.45 micrometer Millipore filter to remove any small hydrocarbon droplets still in suspension. This filtration step is necessary to remove colloidal hydrocarbon and to determine a true water solubility.
Source: Sutton and Calder 1974.
Test substance: Tetradecane (C14 normal paraffin) (629-59-4)
Reliability: (1) valid without restriction
25-JUL-2001 (43)

Value: = .0024 mg/l
GLP: no data
Source: Krop et al 1997.
Test substance: Decylbenzene (104-72-3)
Reliability: (2) valid with restrictions
As cited in HSDB.
25-JUL-2001 (27)

Value: = .035 mg/l at 25 degree C
Method: other: EPIWIN V.3.10
GLP: no data
Test substance: Nonylbenzene (1081-77-2)
Reliability: (2) valid with restrictions
Standard EPA peer-reviewed database and estimation software.
25-JUL-2001

2.6.2 Surface Tension

Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

2.7 Flash Point

Value: ca. 117 degree C
Type:
Method:
Year:
Source: Huntsman Petrochemical Corporation 2000.
Test substance: Alkylate L–210 (Benzene, C6–12 alkyl derivatives; 68608–80–1)
22–OCT–2001 (22)

2.8 Auto Flammability

Value:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

2.9 Flammability

Result:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

2.10 Explosive Properties

Result:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

2.11 Oxidizing Properties

Result:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

2.12 Additional Remarks

Memo: None
01–NOV–2001

3.1.1 Photodegradation

Type: other: Acetonitrite solution
Light source: Sun light
Rel. intensity: = 1 based on Intensity of Sunlight
Conc. of subst.: 2 mg/l at 18 degree C
DIRECT PHOTOLYSIS
Degradation: < 1 % after 14 day
Method: other (measured): EPA
Year: 1979 **GLP:** no
Test substance: other TS: Alkylate 215 (LAB) (67774–74–7)
Method: Test solutions were exposed to natural sunlight for 14 days during the summer (52% possible sunlight). Controls wrapped in aluminum foil were also included. Duplicate photolysis tubes were sacrificed at 0, 2, 5, 9, and 14 days and analyzed by HPLC.
Remark: Greater than 99% of the original material remained at the end of the test period. As natural water solutions were not used, sensitized photolysis tubes were sacrificed at 0, 2, 5, 9, and 14 days and analyzed by HPLC.
Source: Gledhill 1991.
Reliability: (1) valid without restriction
22–OCT–2001 (16)

Type:
DIRECT PHOTOLYSIS
Halflife t1/2: = 7.1 hour(s)
Method: other (calculated): EPIWIN V.3.10
Year: **GLP:** no
Test substance: other TS: Pentadecane (C15 normal paraffin) (629–62–9)
Remark: Hydroxyl radical reaction in air calculated from its estimated rate constant of 1.82 x 10–11 cm cubed/mol–sec at 25 degrees Celcius determined using the structure estimation method of Meylan and Howard.
Source: USEPA and Syracuse Research Corporation 2000.
Reliability: (2) valid with restrictions
Standard EPA peer–reviewed database and estimation software.
22–OCT–2001 (46)

Type:
DIRECT PHOTOLYSIS
Halflife t1/2: = 7.7 hour(s)
Method: other (calculated): EPIWIN V.3.10
Year: **GLP:** no
Test substance: other TS: Tetradecane (C14 normal paraffin) (629–59–4)
Remark: Hydroxyl radical reaction in air calculated from its estimated rate constant of 1.68 x 10–11 cm cubed/mol–sec at 25 degrees Celcius determined using the structure estimation method of Meylan and Howard.
Source: USEPA and Syracuse Research Corporation 2000.
Reliability: (2) valid with restrictions
Standard EPA peer–reviewed database and estimation software.
22–OCT–2001 (46)

Type:
DIRECT PHOTOLYSIS
Halflife t1/2: = 7.5 hour(s)
Method: other (calculated): EPIWIN V.3.10
Year: **GLP:** no
Test substance: other TS: Decylbenzene (104–72–3)
Remark: Hydroxyl radical reaction in air calculated from its estimated rate constant of 1.72 x 10–11 cm cubed/mol–sec at 25 degrees Celcius determined using the structure estimation method of Meylan and Howard.
Source: USEPA and Syracuse Research Corporation 2000.
Reliability: (2) valid with restrictions
Standard EPA peer–reviewed database and estimation software.
22–OCT–2001 (46)

Type:
DIRECT PHOTOLYSIS
Halflife t1/2: = 8.1 hour(s)
Method: other (calculated): EPIWIN V.3.10
Year: **GLP:**
Test substance: other TS: Nonylbenzene (1081–77–2)
Remark: Hydroxyl radical reaction in air calculated from its estimated rate constant of 1.58 x 10–11 cm cubed/mol–sec at 25 degrees Celcius determined using the structure estimation method of Meylan and Howard.
Source: USEPA and Syracuse Research Corporation 2000.
Reliability: (2) valid with restrictions
Standard EPA peer–reviewed database and estimation software.
22–OCT–2001 (46)

3.1.2 Stability in Water

Type:
Method:
Year: **GLP:**
Test substance: other TS: Benzene, C6–12 alkyl derivatives (68608–80–0)
Remark: Stable. Hydrolysis is not expected to occur due to the lack of hydrolyzable functional groups.
03–OCT–2001

3.1.3 Stability in Soil

Type: **Radiolabel:**
Concentration:
Cation exch. capac.
Microbial biomass:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

3.2 Monitoring Data (Environment)

Type of measurement:
Medium:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

3.3.1 Transport between Environmental Compartments

Type:
Media:
Method:
Year:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

3.3.2 Distribution

Media:
Method:
Year:
Remark: Not applicable
03–OCT–2001

3.4 Mode of Degradation in Actual Use

Memo: Biodegradation
03–OCT–2001

3.5 Biodegradation

Type: aerobic
Inoculum: domestic sewage, adapted
Concentration: 20 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: = 67 % after 28 day
Result: readily biodegradable
Kinetic:

7 day	= 0 %
10 day	= 14 %
14 day	= 30 %
25 day	= 65 %
28 day	= 67 %

Method: OECD Guide–line 301 B "Ready Biodegradability: Modified Sturm Test (CO_2 evolution)"
Year: **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Remark: The biodegradation was measured by CO_2 evolution. An emulgator was added to disperse the poorly soluble LAB.
Source: Huls 1987.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.
25–JUL–2001 (18)

Type: aerobic
Inoculum: domestic sewage
Contact time: 28 day
Degradation: = 64 % after 28 day
Result: readily biodegradable
Method: OECD Guide–line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year: **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Source: Istituto Guido Donegani 1995.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.
03–OCT–2001 (25)

Type: aerobic
Inoculum: other: not specified
Concentration: 18 mg/l related to Test substance
Contact time: 35 day
Degradation: = 56 – 61 % after 35 day
Method: other: Shake Flask Carbon Evolution Procedure
Year: 1975 **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Remark: The degradation was less than in other studies, possibly because the test was conducted at LAB concentrations far exceeding the solubility limit. For this reason, studies in more natural systems (Standard River Die–away Test) were carried out using lower LAB concentrations (100–500 ppb) and GC analytical determination. The results show a primary biodegradation of > 90% and a half–life of 4–15 days. Sewage treatment plants remove most of LAB released in sewage. Average percent removals from > 69% to > 98% for trickling filter and activated sludge plants, respectively, are reported.
Source: Gledhill et al 1991.
Reliability: (1) valid without restriction
25–JUL–2001 (16)

Type: aerobic
Inoculum: other: Soil, raw sewage, and activated sludge mixed liquor
Degradation: = 46 % after 35 day
Method: other: Monsanto shake flask procedure
Year: **GLP:** no data
Test substance: other TS: L–210L (Benzene, C6–12 alkyl derivatives; 68608–80–0)
Method: An acclimated inoculum is prepared by the stepwise addition of test compound to a defined medium over a 14–day period. After acclimation, 100 mL of inoculum are mixed with 900 mL of minimal salts media. After aerating the mixture with 70% oxygen in nitrogen, a known quantity of test component is added to each flask. An open reservoir containing 10 mL of 0.15N barium hydroxide is suspended via a glass tube inserted in a neoprene stopper. After sealing, the flasks are agitated in the dark at ambient temperature. Periodic removal and titration of the barium hydroxide solution are used to determine the CO2 evolved. CO2 evolution values obtained with the control are subtracted from values for the test compound.
Remark: The light aromatic naphtha (L–210L) is predominantly a mixture of paraffins, alkylbenzene, and indanes. The CO2 evolution of 46% of theory probably arises from degradation of the paraffin and alkybenzene components. The L–210L tested (in 1980) consisted of 29% paraffin, 44% alkylbenzene, 24% indanes, with an avg.C # = 13.5. Because of advances in the production process, the current composition is approximately 40% paraffins and 60% alkylbenzenes. Therefore, this study likely under predicts the actual biodegradation of the current product.
Source: Saeger 1980.
Reliability: (1) valid without restriction
25–JUL–2001 (29) (38)

Type: aerobic
Inoculum: other: Enriched sediment medium
Degradation: = 75 % after 8 day
Method: other: Experimental conditions have been devised to accelerate the processes of degradation of hydrocarbons in sediments.
Year: **GLP:** no data
Test substance: other TS: Pentadecane (C15 normal paraffin) (629–62–9)
Method: Sediments previously freed from all organic matter were used. After drying, these sediments were mixed with pentadecane. The material was then incubated for 8 days in a medium containing an initial bacterial MLP inoculum of 1x10E+8 cells/g of sediment. At the end of the incubation period the sediment was harvested and extracted. The FA fraction was analyzed.
Remark: The experimental conditions make it possible to determine the correlations between bacterial activity and the accumulation of petroleum constituents and so lead to a better knowledge of the potentialities of auto–purification of the marine medium.
Source: Azoulay et al 1983.
Reliability: (2) valid with restrictions
02–NOV–2001 (3)

Type: aerobic
Inoculum:
Degradation: 100 % after 56 day
Method:
Year: **GLP:**
Test substance: other TS: Pentadecane (C15 normal paraffin) (629–62–9)
Method: Heated crude oil was added to a concentration of 1 g/L to a natural seawater medium. This solution was cultivated at 20 degrees Celcius under constant shaking (100 strokes/min) to promote the growth of indigenous oil–degrading microorganisms. The abundance of approximately 50 constituent compounds was determined using GC–MS in SIM mode after 8 weeks.
Remark: Pentadecane was 100% biodegraded within 8 weeks.
Source: Dutta and Harayama 2000.
Reliability: (1) valid without restriction
25–JUL–2001 (12)

Type: aerobic
Inoculum:
Degradation: 100 % after 56 day
Method:
Year: **GLP:**
Test substance: other TS: Tetradecane (C14 normal paraffin) (629–59–4)
Method: Heated crude oil was added to a concentration of 1 g/L to a natural seawater medium. This solution was cultivated at 20 degrees Celcius under constant shaking (100 strokes/min) to promote the growth of indigenous oil–degrading microorganisms. The abundance of approximately 50 constituent compounds was determined using GC–MS in SIM mode after 8 weeks.
Remark: Tetradecane was 100% biodegraded within 8 weeks.
Source: Dutta and Harayama 2000.
Reliability: (1) valid without restriction
25–JUL–2001 (12)

Type:
Inoculum:
Result: other: Biodegrades easily
Method: other: No data
Year: **GLP:** no data
Test substance: other TS: Tetradecane (C14 normal paraffins) (629–59–4)
Remark: Tetradecane was listed as a compound that biodegrades and was classified in level 2 (degraded without much difficulty) in a 5–tiered rating system on ease of biodegradability.
Source: Abrams et al 1975.
Reliability: (2) valid with restrictions
As cited in HSDB.
25–JUL–2001 (1)

Type: aerobic
Inoculum: other: Enriched sediment medium
Degradation: = 72 % after 8 day
Method: other: Experimental conditions have been devised to accelerate the processes of degradation of hydrocarbons in sediments.
Year: **GLP:** no data
Test substance: other TS: Nonylbenzene (1081–77–2)
Method: Sediments previously freed from all organic matter were used. After drying, these sediments were mixed with nonylbenzene. The material was then incubated for 8 days in a medium containing an initial bacterial MLP inoculum of 1x10E+8 cells/g of sediment. At the end of the incubation period the sediment was harvested and extracted. The FA fraction was analysed.
Remark: The experimental conditions make it possible to determine the correlations between bacterial activity and the accumulation of petroleum constituents and so lead to a better knowledge of the potentialities of auto–purification of the marine medium.
Source: Azoulay et al 1983.
Reliability: (2) valid with restrictions
03–OCT–2001 (3)

Type: aerobic
Inoculum: other: Alcaligenes sp. PHY12 originating from a mixed bacterial community isolated from seafoam
Degradation: = 65 % after 10 day
Method:
Year: **GLP:** no data
Test substance: other TS: Nonylbenzene (1081–77–2)
Method: Pyrex flasks containing 120 mL of medium composed of seawater supplemented with yeast extract, ammonium chloride, sodium phosphate and n–nonylbenzene were used. Aeration was realized with strong agitation at 30 degrees Celcius on a reciprocal shaker (96 rpm). Traces of anthraquinone were added as a photosensitivity agent.
Remark: The reported degradation value is for biodegradation alone. Concurrent studies demonstrate that in the presence of light, photo–oxidation of the more refractory biodegradation products results in even greater total degradation (84% in 10 days).
Source: Rotani 1987.
Reliability: (1) valid without restriction
22–OCT–2001 (37)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: Not a High Production Volume Challenge Program endpoint.
01–NOV–2001

3.7 Bioaccumulation

Species:
Exposure period:
Concentration:
BCF:
Elimination:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
01–NOV–2001

3.8 Additional Remarks

Memo: None
01–NOV–2001

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: other: Static daily renewal
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 14 day
Unit: mg/l **Analytical monitoring:** yes
LC50: > .0055
Method: other: OECD Guideline 202
Year: 1984 **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Method: The LAB tested was comprised of 93% alkylbenzenes and 18% phenylalkanes. The relative percentage of the C10–13 homologues is 14:34:31:21, respectively. The treatment solutions were prepared by adding 5 g of LAB to 5 L of reconstituted water. After being vigorously stirred for 24 hours and allowed to stand for 4 hours, the aqueous phase was separated and filtered. This solution was the solubility concentration and was used in the experiment. In addition to the undiluted concentration, two more test concentrations were obtained by 2:1 and 1:1 dilutions with reconstituted water. Test solutions were renewed daily.
Remark: No toxic effects were observed. Measured concentrations in the undiluted sample at the beginning of the study ranged from 0.0046 to 0.0065 mg/L (mean=0.0055).
Source: Calcinai et al 2001.
Reliability: (1) valid without restriction
03–OCT–2001 (6)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: > 1000
Method: other: EPA–660/3–7–009: Method for acute toxicity tests with fish, macroinvertebrates and amphibians.
Year: 1975 **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Remark: The test shows no adverse effects after 96 hours at nominal concentration (1000 mg/L) up to and exceeding the water solubility using a solvent carrier. Rainbow trout and fathead minnows were also tested with the same results.
Source: Gledhill et al 1991.
Reliability: (1) valid without restriction
03–OCT–2001 (16)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50: > 1000
Method: other: Bestimmung der Wirkung von wasserinhaltsstoffen auf Fische, DIN 38412 Teil 15
Year: 1982 **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Remark: This test shows no adverse effects after 48 hours at nominal concentration (1000 mg/L) up to and exceeding the water solubility using an emulsifier.
Source: Huls 1994.
Reliability: (2) valid with restrictions
Reported in LAB Risk Assessment document.
25–JUL–2001 (19)

Type: flow through
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 21 day
Unit: mg/l **Analytical monitoring:** yes
LC50: > .079
Method: OECD Guide–line 203 "Fish, Acute Toxicity Test"
Year: 1992 **GLP:** yes
Test substance: other TS: Phenyl–C10 (C10 LAB) and LAB (67774–74–7)
Remark: Fish were exposed to duplicate chambers of a single concentration (limit test) in a flow through system. Acetone was used as a solvent. The mean measured concentrations were 0.058 and 0.079 mg/L for the LAB and phenyl C–10, respectively. These assayed concentrations were higher than water solubility limits.
The exposure period lasted up to 3 weeks.
Result: No toxic effects were observed.
Source: Fernandez et al 2000.
Reliability: (1) valid without restriction
03–OCT–2001 (14)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: > 1000
Method: other: Methods of acute toxicity tests with fish, macroinvertebrates, and amphibians
Year: 1975 **GLP:** yes
Test substance: other TS: L210–L (Benzene, C6–12 alkyl derivs.; CAS # 68608–80–0)
Remark: No adverse effects were observed after 96 hours at nominal concentrations up to 1000 mg/L. Acetone was used as a solvent to enhance solubility.
Source: Thompson and Griffen 1981.
Reliability: (2) valid with restrictions
25–JUL–2001 (44)

Type: flow through
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 7 day
Unit: mg/l **Analytical monitoring:** yes
NOEC: > 1240
Method:
Year: 1983 **GLP:** yes
Test substance: other TS: Tetradecane (C14 normal paraffin) (629–59–4)
Method: Rainbow trout were fed experimental diets containing a mixture of n–paraffins. Fish were fed twice a day (at 0900 h and 1630 h) for seven days. Feces were recovered automatically and the relative absorption of different carbon chain lengths was measured. All fish were maintained at 14 degrees Celcius in a 50 liter aquaria under a constant flow of 4 L/min and a 12 hour photoperiod.
Remark: No mortality was observed in the study.
Source: Cravedi 1983.
Reliability: (1) valid without restriction
03–OCT–2001 (9)

Type: flow through
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 7 day
Unit: mg/l **Analytical monitoring:** yes
NOEC: > 2110
Method:
Year: 1983 **GLP:** yes
Test substance: other TS: Pentadecane (C15 normal paraffin) (629–62–9)
Method: Rainbow trout were fed experimental diets containing a mixture of n–paraffins. Fish were fed twice a day (at 0900 h and 1630 h) for seven days. Feces were recovered automatically and the relative absorption of different carbon chain lengths was measured. All fish were maintained at 14 degrees Celcius in a 50 liter aquaria under a constant flow of 4 L/min and a 12 hour photoperiod.
Remark: No mortality was observed in the study. The maximum digestibility of all n–paraffins tested was observed for pentadecane.
Source: Cravedi 1983.
Reliability: (1) valid without restriction
02–NOV–2001 (9)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
NOEC: > .013
EC50: > .013
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: **GLP:** yes
Test substance: other TS: A commercial LAB produced in an HF alkylation process (67774–74–7)
Method: The LAB tested was comprised of 93% alkylbenzenes and 18% phenylalkanes. The relative percentage of the C10–C13 homologues is 14:34:31:21, respectively. The treatment solutions were prepared by adding 5 g of LAB to 5 L of reconstituted water. After being vigorously stirred for 24 hours and allowed to stand for 4 hours, the aqueous phase was separated and filtered. This solution was the solubility concentration and was used in the experiment. Measured concentrations at the end of the 48–hour study were 0.010 to 0.013 mg/L.
Remark: No effects of immobilization were observed at the solubility concentration.
Source: Calcinai et al 2001.
Reliability: (1) valid without restriction
03–OCT–2001 (6) (47)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: > .04
Method: OECD Guide–line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: other TS: A commercial LAB produced in an HF alkylation process (67774–74–7)
Remark: Separate tests were conducted with LAB dissolved in acetone and LAB without solvent. In the first test, acetone–assisted concentrations of 0.05, 0.1, 0.2, 0.4, 0.8, 1.0, 1.2, and 1.4 mg/L were prepared. In the second test, a saturated LAB solution (0.040 mg/L) was tested as is and diluted to 0.030, 0.020, 0.010, and 0.005 mg/L. Results of the first test show that LAB is not toxic to Daphnia at the limit of solubility. In the second test the EC50 was 1.1 mg/L, which is much higher than the solubility concentration.
Source: Verge at al 1999.
Reliability: (1) valid without restriction
03–OCT–2001 (47)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: > .1
Method: OECD Guide–line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: **GLP:** no data
Test substance: other TS: Phenyl–C10 (C10 LAB)
Remark: A distinction was made between immobilized and effected. No effects were observed up to 48 hours. The study was extended out to 144 hours and the EC50s were 0.083 at 96 hours, 0.035 at 120 hours, and 0.025 at 144 hours. The results show that the absence of toxicity can be related to the limited exposure period. If the exposure time is expanded up to 5 days, the EC50 values for waterborne exposures reach the solubility level. This hypothesis is clearly consistent with the assumption of non–polar narcosis as mode of action and toxicity related to the total body burden of LAB. Due to the low water solubility, prolonged waterborne exposures are required to reach the lethal body burden, as has been demonstrated for other poorly soluble hydrocarbons.
Source: Fernandez et al 2000.
Reliability: (1) valid without restriction
03–OCT–2001 (15)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: > 1000
Method: other: EPA 600/9–78–018 The Selenastrum capricornutum Printz algal assay
Year: 1978 **GLP:**
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Remark: Selenastrum capricornutum is not affected after 96 hours at nominal concentration (1000 mg/L) up to and exceeding the water solubility with a solvent carrier.
Source: Gledhill et al 1991.
Reliability: (1) valid without restriction
25–JUL–2001 (16)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:**
EC50: > .1
Method: OECD Guide–line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:**
Test substance: other TS: LAB (67774–74–7) and individual homologues (phenyl C8, phenyl C10, phenyl C12, phenyl C14)
Remark: LAB concentrations tested were 0.025, 0.050, and 0.100 mg/L. No inhibition of growth was observed for LAB or any of the individual homologues.
Source: Moreno et al 2000.
Reliability: (1) valid without restriction
03–OCT–2001 (33)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type:
Species:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species:
Endpoint:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–20
01

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species:
Endpoint:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint. 03–OCT–2001

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type:
Species:
Endpoint:
Exposure period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint. 03–OCT–2001

4.6.2 Toxicity to Terrestrial Plants

Species:
Endpoint:
Expos. period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint. 03–OCT–2001

4.6.3 Toxicity to other Non–Mamm. Terrestrial Species

Species:
Endpoint:
Expos. period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint. 03–OCT–2001

4.7 Biological Effects Monitoring

Memo: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

4.8 Biotransformation and Kinetics

Type:
Remark: Not a High Production Volume Challenge Program endpoint.
03–OCT–2001

4.9 Additional Remarks

Memo: None
03–OCT–2001

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex: male/female
Number of Animals:
Vehicle: other: none
Value: > 5000 mg/kg bw
Method: other: OECD Guide–line 401: Rats were given a single oral administration by gavage.
Year: **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7). Average side chain length of 11.1 to 11.8.
Remark: No deaths were observed. Pilo–erection was observed shortly after dosing in all treated rats.
Source: Huntingdon Research Centre 1984.
Reliability: (2) valid with restrictions
Data as reported in LAB Risk Assessment, revised June 1997.
25–JUL–2001 (21)

Type: LD50
Species: rat
Sex: male/female
Number of Animals: 5
Vehicle:
Value: > 10000 mg/kg bw
Method: other: Undiluted test material was provided to three male and two female rats in a single oral dose.
Year: 1978 **GLP:** no data
Test substance: other TS: L–210H and L–210L (68608–80–0)
Remark: No signs of toxicity were observed with the exception of some weight loss on one to two days. Viscera were normal after 14 days. An earlier study by the same laboratory (1973) tested at a higher dose resulted in an LD50 > 15,800 mg/kg bw.
Source: Younger Laboratories 1978.
Reliability: (2) valid with restrictions
03–OCT–2001 (50)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value: > 1.82 mg/l
Method: other
Year: **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7). Average side chain length of 11.1 to 11.8.
Method: The substance was administered as an aerosol containing > 90% particles with diameter less than 10 microns.
Remark: No deaths were observed.
Source: Monsanto 1982.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision. Original report not reviewed.
25–JUL–2001 (31)

Type: LC50
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value: = 71 mg/l
Method: other
Year: **GLP:** no data
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Method: The substance was administered as an aerosol.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision. Original report not reviewed.
25–JUL–2001 (45)

Type: LC50
Species: rat
Sex: male
Number of Animals: 6
Vehicle: other: none
Exposure time: 6 hour(s)
Value: > .9 mg/l
Method:
Year: 1973 **GLP:** no data
Test substance: other TS: Benzene C6–12 alkyl derivs. (68608–80–0)
Method: A.T.S. Sprague–Dawley albino male rats were exposed in a 35 L inhalation chamber for 6 hrs at 27 degrees Celcius. The air flow rate was 4.0 L/min.
Remark: Four studies were performed with the same results. The concentrations of test substance in the different studies were 0.9, 0.55, 0.3, and 0.34 mg/L.

Result: No significant toxic signs were observed in any of the studies. Viscera appeared normal after 14 days.
Source: Younger Laboratories 1973; Younger Laboratories 1978.
Reliability: (2) valid with restrictions
03–OCT–2001 (49) (50)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rat
Sex: male/female
Number of Animals:
Vehicle: no data
Value: > 2000 mg/kg bw
Method: OECD Guide–line 402 "Acute dermal Toxicity"
Year: **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7). Average side chain length of 11.1 to 11.8.
Result: After a single dermal administration in rats, no deaths were observed, no signs of systemic toxicity were observed, and terminal autopsy findings were normal.
Source: Huntingdon Research Centre 1984.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.
25–JUL–2001 (20)

Type: LD50
Species: other: New Zealand Albino Rabbits
Sex: male/female
Number of Animals: 7
Vehicle: no data
Value: > 1260 mg/kg bw
Method:
Year: **GLP:** no data
Test substance: other TS: Benzene, C6–12–alkyl derivs. (68608–80–0) (L–210H)
Method: One male or female was exposed dermally to six doses (794, 1000, 1260, 2000, 3160, 5110 mg/kg) of undiluted test substance for 24 hours. The animals were observed for 14 days.
Result: All animals exposed to doses up to 1260 mg/kg survived. Mortality occurred for animals exposed to doses of 2000 mg/kg and higher. Weight loss was observed at two through six days in survivors. Animals in the higher concentrations experienced increasing weakness, collapse, and death. Gross autopsy of the decendents included lung and liver hyperemia, enlarged gallbladder, darkened kiddneys, and gastrointestinal inflammation. Viscera appeared normal in the surviving animals.
Source: Younger Laboratories 1978.
Reliability: (2) valid with restrictions
03–OCT–2001 (50)

Type: LD50
Species: other: New Zealand Albino Rabbits
Sex: male/female
Number of Animals: 4
Vehicle: no data
Value: > 2000 mg/kg bw
Method: other: One male or one female was exposed dermally to four doses (1260, 2000, 3160, 5010 mg/kg) of undiluted test substance for 24 hours. The animals were observed for 14 days.
Year: **GLP:** no data
Test substance: other TS: Benzene, C6–12–alkyl derivs. (68608–80–0) (L–210L)
Result: All animals exposed to doses up to 2000 mg/kg survived while mortality occurred for animals exposed to the two highest doses. Weight loss was observed at two to four days in survivors. Animals in the higher concentrations experienced increasing weakness, collapse, and death. Gross autopsy of the decendents included lung and liver hyperemia, enlarged gallbladder, darkened kiddneys, and gastrointestinal inflammation. Viscera appeared normal in the surviving animals.
Source: Younger Laboratories 1978.
Reliability: (2) valid with restrictions
25–JUL–2001 (50)

Type: LD50
Species: other: New Zealand Albino Rabbits
Sex: male/female
Number of Animals: 4
Vehicle: no data
Value: > 5010 mg/kg bw
Method: other: One male or one female rabbit was exposed to three doses (3160, 5010, 7940 mg/kg) of the undiluted test substance for 24 hours. The animals were observed for 14 days.
Year: **GLP:** no data
Test substance: other TS: Benzene, C6–12–alkyl derivs. (68608–80–0) (L210H + L210L)
Result: Animals exposed to 3160 and 5010 mg/kg survived. Female and male rabbits exposed to the 7940 mg/kg dose died on days 2 and 10, respectively. Signs of intoxication included reduced appetite and activity (days four to seven in survivors), increasing weakness, collapse, and death. Gross autopsy of the decendents revealed hemorrhagic lungs, mottled and discolored liver, enlarged gallbladder, and gastrointestinal inflammation. Viscera in the survivors appeared normal.
Source: Younger Laboratories 1973.
Reliability: (2) valid with restrictions
03–OCT–2001 (48) (49)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.v.
Value: = 3493 mg/kg bw
Method:
Year: **GLP:** no data
Test substance: other TS: Pentadecane (C15 normal paraffin) (629–62–9)
Source: Louis 1996.
Reliability: (4) not assignable
25–JUL–2001 (28)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species:
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result:
EC classificat.:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
01–NOV–2001

5.2.2 Eye Irritation

Species:
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
01–NOV–2001

5.3 Sensitization

Type:
Species:
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
01–NOV–2001

5.4 Repeated Dose Toxicity

Species: rat **Sex:** male/female
Strain: Sprague–Dawley
Route of admin.: inhalation
Exposure period: 70 day(s) (14 week period)
Frequency of treatment: 6 hours per day/5 days per week
Post. obs. period:
Doses: 0, 102, 298, or 580 mg LAB per cubic meter of air in 10m3 inhalation chambers
Control Group: yes, concurrent no treatment
NOAEL: = 102 ppm
Method: other: EPA/TSCA.
Year: **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Method: 15 male and 15 female rats were exposed per group.
Remark: Skin and mucous membrane irritation and respiratory problems were evident at the mid– and high exposure concentrations. Body weight gains were also depressed at these levels. While liver weights and serum levels of hepatic enzymes were elevated in females from the high concentrations, there were no gross or histopathological changes.
Source: Monsanto 1986.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.
25–JUL–2001 (32)

Species: rat **Sex:**
Strain: no data
Route of admin.: oral feed
Exposure period: 4 weeks
Frequency of treatment: daily in diet
Post. obs. period:
Doses: various concentrations up to 20000 ppm (2%)
Control Group:
LOAEL: = 125 mg/kg bw
Method: other: EPA/TSCA
Year: **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Remark: Reduction in body weight and food consumption were observed at all exposure levels. No gross pathological changes were noted. Histopathology was not carried out. The lowest dose tested was 2500 ppm, which corresponds to 125 mg/kg bw.
Source: Monsanto.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.
25–JUL–2001 (30)

Species: mouse **Sex:**
Strain:
Route of admin.:
Exposure period: 20 weeks
Frequency of treatment:
Post. obs. period:
Doses:
Control Group:
LOAEL: = 9600 mg/kg
Method:
Year: **GLP:**
Test substance: other TS: Tetradecane (629–59–4)
Remark: Patty’s reports this result as "the lowest toxic dose (TDLo) of tetradecane for mice is 9600 mg/kg for 20 weeks." No further information is provided and Patty’s lists only an incorrect citation. Therefore, then reliability of this value cannot be determined.
Source: Sandmeyer 1981.
Reliability: (4) not assignable
08–NOV–2001 (39)

5.5 Genetic Toxicity 'in Vitro'

Type: Bacterial reverse mutation assay
System of testing: Salmonella typhimurium TA 1535, TA 100, TA 1537, and TA 98
Concentration: 0, 100, 1000, 4000, 8000, and 10000 ug/plate
Metabolic activation: with and without
Result: negative
Method: Directive 84/449/EEC, B.14 "Other effects – Mutagenicity (Salmonella typhimurium – reverse mutation assay)"
Year: 1984 **GLP:** no data
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Source: Bronzetti et al 1991.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.
01–NOV–2001 (4)

Type: Mammalian cell gene mutation assay
System of testing: Chinese Hamster Ovary (CHO) cells
Concentration: 100 to 2000 micrograms/mL
Metabolic activation: with and without
Result: negative
Method: other: EPA/TSCA
Year: **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Remark: V79/HGPRT and Saccharomices cerevisiae genetic toxicity studies conducted on LAB by other authors also showed negative results.
Result: There were no statistically significant increases in mutation frequencies for the substance compared to the negative control. Cytotoxicity was significant at and above 1250 micrograms/mL with and without metabolic activation.
Source: Robinson and Nair 1992.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.
25–JUL–2001 (35)

Type: Bacterial reverse mutation assay
System of testing: Salmonella typhimurium TA 1535, TA 100, TA 1537, and TA 98
Concentration: .03, 12, 60, 300, 1000, 3000 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: EPA/TSCA
Year: **GLP:** yes
Test substance: other TS: Benzene C10–13 alkyl derivs. (LAB) (67774–74–7)
Remark: The highest concentration produced evidence of either toxicity or insolubility.
Source: Robinson and Nair 1992.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997

revision.
02–NOV–2001 (35)

5.6 Genetic Toxicity 'in Vivo'

Type: other: Bone marrow chromosome aberration assay
Species: rat **Sex:** male/female
Strain: Sprague–Dawley
Route of admin.: gavage
Exposure period: single treatment
Doses: 1200, 4000, and 12700 mg/kg bw
Result: negative
Method: other: EPA/TSCA – Bone marrow chromosome aberration
Year: 1992 **GLP:** yes
Test substance: other TS: LAB undiluted or dissolved in corn oil (67774–74–7)
Result: A significant mean body weight loss was found in the groups treated with the highest dose. No statistically significant increases in chromosomal aberration or gaps were observed in the treated groups in any of the sampling times. Both mean chromosome numbers and mean mitotic indices were similar in test and vehicle control groups.
Source: Robinson and Nair 1992.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.
25–JUL–2001 (35)

5.7 Carcinogenicity

Species: **Sex:**
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Post. obs. period:
Doses:
Result:
Control Group:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
01–NOV–2001

5.8 Toxicity to Reproduction

Type: Two generation study
Species: rat **Sex:**
Strain: other: CD (Charles River Breeding Laboratories)
Route of admin.: gavage
Exposure Period: 35 weeks
Frequency of treatment: single daily dose
Premating Exposure Period
male: 10 weeks
female: 10 weeks
Duration of test: 35 weeks
Doses: 0, 5, 50, and 500 mg/kg/d
Control Group:
NOAEL Parental: = 50 mg/kg bw
NOAEL F1 Offspr.: = 50 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: other TS: linear alkylbenzene in corn oil (67774–74–7)
Method: Four groups of 30 male and 30 female were given the test substance by gavage once daily for about 10 weeks before mating. Once mated (as evidence by a copulatory or sperm in the vaginal smear), females were housed separately for the remainder of gestation. Females were dosed during mating, gestation and lacation for a total of 127 days of treatment. After wenning, 30 males and 30 females of the F1 generation were dosed for an 11–week premating period. Dosing of F1 females continued through mating, gestation, and lactation. All of the resulting F2 pups were euthanized on day 13 of gestation.
Remark: All adults and pups received a gross post–mortem examination. Histopathology studies were conducted on reproductive tissues, tissues with gross lesions, and the pituitary gland taken from each adult in the control and high dose groups.
Result: There was evidence of toxicity in adults and offspring at the 500 mg/kg/day dose level, with the most consistent effects being depressed weight gains in adults, smaller litters, and fewer live pups; decreased pup survival and lower pup survival at some intervals. At 50 mg/kg/day, only a reduction in F1 of pup weight gain on day 7 was observed, but this effect had returned to normal at days 14 and 21. This temporary reduction in pup weight occurred in on generation, and this was not consistent across generations. Based on the significant effects at 500 mg/kg/day and the non consistent effects at the lower dose, the NOAEL for reproductive toxicity is 50 mg/kg/day for both parental and neonatal animals.
Source: Robinson and Nair 1992.
Reliability: (2) valid with restrictions
03–OCT–2001 (35)

5.9 Developmental Toxicity/Teratogenicity

Species: rat **Sex:** female
Strain: other: CD (Charles River Breeding Laboratories)
Route of admin.: gavage
Exposure period: days 6–15 of gestation
Frequency of treatment: single daily dose
Duration of test: 20 days
Doses: 125, 500, and 2000 mg/kg bw/day
Control Group:
NOAEL Maternalt.: = 125 mg/kg bw
Method: other
Year: **GLP:** yes
Test substance: other TS: Alkylate 215 (68648–87–3) as a surrogate for LAB (67774–74–7)
Method: Groups of 24 mated rats were given the test substance in corn oil on days 6–15 of gestation. Rats were observed twice daily and the body weights recorded on gestation days 0, 6, 10, 12, 15, and 20. Fetuses were delivered by caesarean section on gestation day 20 and the numbers of live, dead, and researched fetuses, total implantations, and corpora lutea were recorded. Fetuses and surviving mated females received post mortem examinations.
Remark: The substance should not be considered as a developmental toxicant since an increased incidence of ossification variations and delayed ossification only at dose levels including maternal toxicity cannot be considered as specific effects on prenatal development.
Result: Depressed maternal food consumption and weight gains were observed at 500 mg/kg/day and 2000 during treatment , but significantly increased in the post treatment period. No treatment–related increases in soft tissue malformations and variations were observed in either the maternal or fetal generations. Some skeletal malformations (wavy ribs) and ossification variations were observed in the highest doses.
Source: Robinson and Schroeder 1992.
Reliability: (1) valid without restriction
03–OCT–2001 (36)

5.10 Other Relevant Information

Type:
Remark: None
03–OCT–2001

5.11 Experience with Human Exposure

Memo: None
03–OCT–2001

(1) Abrams, E.F. et. al. 1975. Indentification of organic compounds in effluents from industrial sources. USEPA–560/3–75–002, as cited in HSDB.

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7.1 Risk Assessment

Memo: Refer to LAB Alkylate Top Assessment Plan
01–NOV–2001